NASA-CR-199357

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PDF METHODS FOR COMBUSTION IN HIGH-SPEED TURBULENT FLOWS

Second Annual Technical Report

Grant NAG-1-1542

from

NASA Langley Research Center
Dr. J. P. Drummond

to

Cornell University
Ithaca, New York 14853

Period: August 25, 1994 - August 24, 1995
Principal Investigator: Professor Stephen B. Pope

September 6, 1995

(NASA-CR-199357) PDF METHODS FOR COMBUSTION IN HIGH-SPEED TURBULENT FLOWS Annual Technical Report No. 2, 25 Aug. 1994 - 24 Aug. 1995 (Cornell Univ.) 12 p

N96-10806

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INTRODUCTION

This report describes the research performed during the second year of this three-year project. The ultimate objective of the project is to extend the applicability of pdf methods from incompressible to compressible turbulent reactive flows.

As described in subsequent sections, progress has been made on:

1. formulation and modelling of pdf equations for compressible turbulence, in both homogeneous and inhomogeneous inert flows,

2. implementation of the compressible model in various flow configurations, namely decaying isotropic turbulence, homogeneous shear flow and plane mixing layer.

PERSONNEL

The work is being performed by the Ph.D. student Bertrand Delarue as well as by the P.I. Stephen Pope and the co-P.I. David Caughey. During the reporting period, Delarue and Pope visited NASA Langley to discuss the research with Dr. Drummond and others. Having passed both the Ph.D. qualifying examination and the "Admission to Candidacy" examination, Bertrand Delarue has essentially completed all the requirements for the Ph.D. except for research.

PDF MODELLING OF COMPRESSIBLE TURBULENCE

In inert high-speed compressible flows, it is necessary to include two thermodynamic variables in the usual velocity-dissipation pdf formulation. The choice of such variables has been reviewed in Delarue and Pope (1994). We decided to take the pressure p and the specific internal energy e as the two thermodynamic state variables. Based on physics, and guided by existing models representing such phenomena as the compressible dissipation and the pressure-dilatation correlation, we developed stochastic model equations for

the two state variables and modified the existing model equation for the velocity.

As it is now being used, the PDF model consists of four sets of equations:

1. the Simplified Langevin Model for the velocity (Haworth & Pope 1986),
2. a new model for the turbulent frequency $\omega = \varepsilon/k$, ε being the dissipation rate and k the turbulence kinetic energy (Pope 1994),
3. a model equation for e based on the First Law of thermodynamics,
4. a model equation for p based on mass conservation and on Zeman's model (Zeman 1991) for the pressure-dilatation correlation.

As will be shown in the next sections, this model has been successfully applied to simple homogeneous and inhomogeneous flows.

HOMOGENEOUS FLOWS

The main objective of this part of the work is to assess the accuracy of the pressure-dilatation modelling. As mentioned above, the model equation for pressure has been designed to include Zeman's model for the pressure-dilatation correlation. However, due to the stochastic formulation of the model equations, the second moment equations are not strictly identical to Zeman's. We therefore compared our model in the frame of a particle code to Zeman's model in the frame of a second-order closure, in both decaying isotropic turbulence, and initially isotropic turbulence subjected to a constant mean shear.

In the decaying isotropic turbulence case, we compared the models under different sets of initial conditions, namely at different turbulent Mach numbers M_{t0} and levels of pressure fluctuations Π_0, to reproduce the exchange between turbulence kinetic energy and pressure energy represented by the pressure-dilatation correlation. As can be seen from Figs. 1 and 2, our model compares well with Zeman's.

In the homogeneous shear case, we compared our results to DNS by Sarkar, Erlebacher and Hussaini (1991). The good result of Fig. 3 is to be considered with much care, due to the simplicity of the models used.

In addition to developing a specific model, we have developed a methodology to relate second-order closures to PDF methods. Consequently, any improvements in second-order closures made by other research groups can readily be incorporated in our PDF model.

INHOMOGENEOUS FLOWS: PLANE MIXING LAYERS

A central issue in particle methods used to solve PDF equations is the determination of the mean pressure. As of last year, three approaches were being pursued: the Converging Field Algorithm (CFA), Smooth Particle Hydrodynamics (SPH) and a Pressure-Velocity Correction algorithm (PVC). Of these only SPH had been successfully applied to compressible flows. For our compressible model, we have a new approach: we can use the mean pressure obtained from the averaging of the particle thermodynamic pressure p. This method has been investigated and deemed unsatisfactory, because the pressure field obtained under such conditions is extremely noisy, essentially because of statistical error. We thus decided that it was necessary to couple our compressible model with a pressure algorithm in order to reduce the level of noise in the pressure field for inhomogeneous flows. The first step was to choose the pressure algorithm.

Pope (1994) has written a particle code PDF2DV to obtain a solution to the modelled PDF equations, which uses the PVC algorithm. This code has been tested in the case of a temporally evolving mixing layer, in the incompressible case. The goals of this testing were to evaluate the accuracy of the new turbulent frequency model, to test PVC in incompressible flows and to gain overall confidence in the new code. Results have been compared to DNS by Rogers & Moser (1994) and experiments by Bell & Mehta (1990). As one can see from Figs. 4 and 5, the PDF results compare extremely well with the data.

We then proceeded to work out in detail the coupling between our compressible model and PVC. It is necessary to modify the model equations to achieve this coupling, because with the mean pressure being obtained by PVC, it is no longer necessary to compute it at the particle level. The formulation of the problem is thus slightly altered: instead of the total pressure,

we compute the fluctuating pressure $p' = p - \langle p \rangle$ at the particle level, and the mean pressure using PVC. It is then straightforward to compute the total pressure by adding the two. The main features of the model (pressure-dilatation model, pressure variance transport equation) are unaltered by this modification.

Results of our model in a plane compressible turbulent mixing layer are shown in Figs. 6-9. The fluids in each stream have identical thermodynamic properties, and the convective Mach number is about 0.13. The effects of compressibility on the mean flow and on the turbulence are thus fairly low: the maximum turbulent Mach number is approximately 0.025 in the self-similar region. As one can see, the fields are smooth. The main features of a compressible mixing layer are present: the internal energy increases in the turbulent region, essentially because of dissipation, while the density and the pressure decrease. The adverse streamwise pressure gradient is due to the presence of frictionless walls: we are not dealing here with an ideal free shear layer. For the same reason the density in the non-turbulent region is increasing in the streamwise direction.

FUTURE WORK

The next step in the research program is to test the compressible model at different Mach numbers, to try to reproduce the well-known decrease in the mixing layer spreading rate with increasing compressibility. We will also study the effect of density gradients on the statistics of the flow.

Then, the model will be modified to account for reaction, at first by assuming fast chemistry. Finally, realistic simplified hydrogen/air chemistry will be incorporated in order to study reacting compressible shear layers for which there are experimental data.

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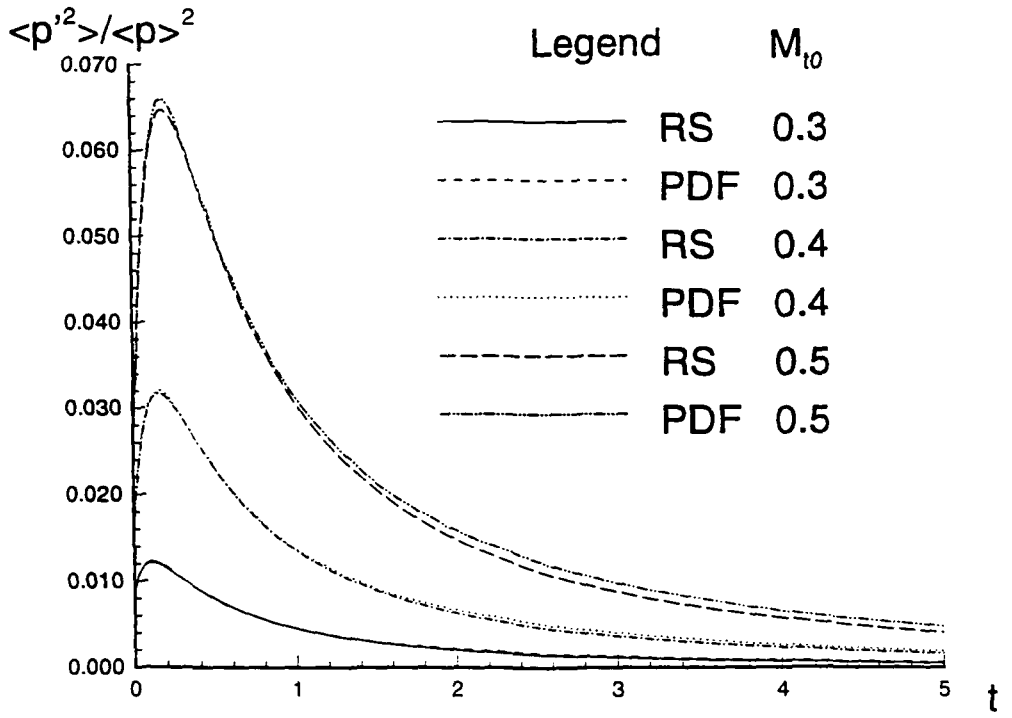

Fig. 1 (a). Comparison of normalized pressure variance values for the Reynolds stress closure (RS) and the PDF method (PDF). $\Pi_0 = 0.05$, the values of M_{t0} are given on the plot.

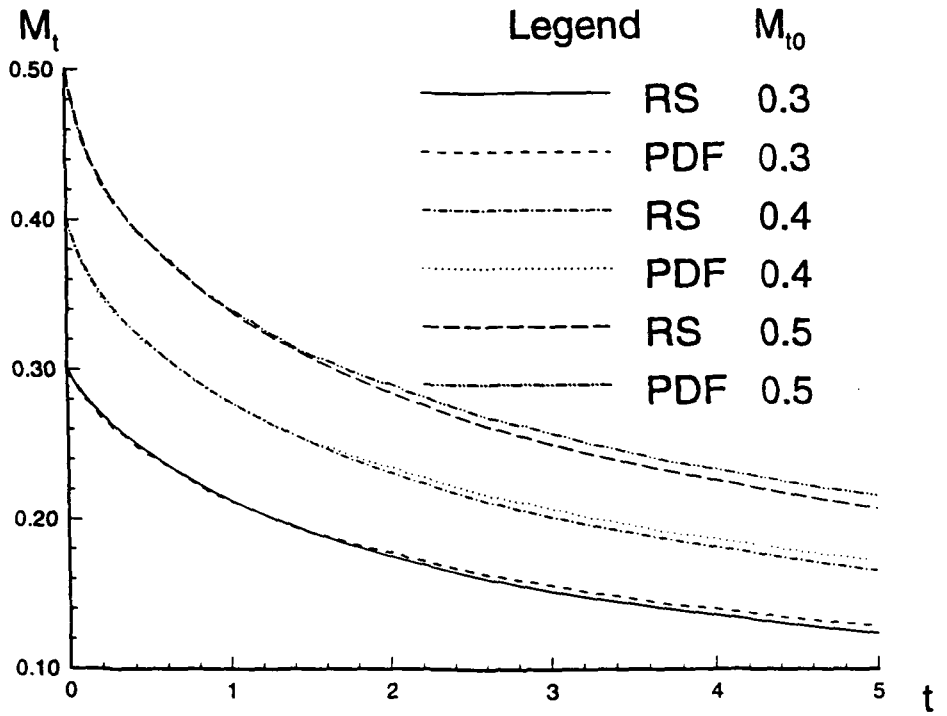

Fig. 1 (b). Comparison of turbulent Mach number values for the Reynolds stress closure (RS) and the PDF method (PDF). $\Pi_0 = 0.05$, the values of M_{t0} are given on the plot.

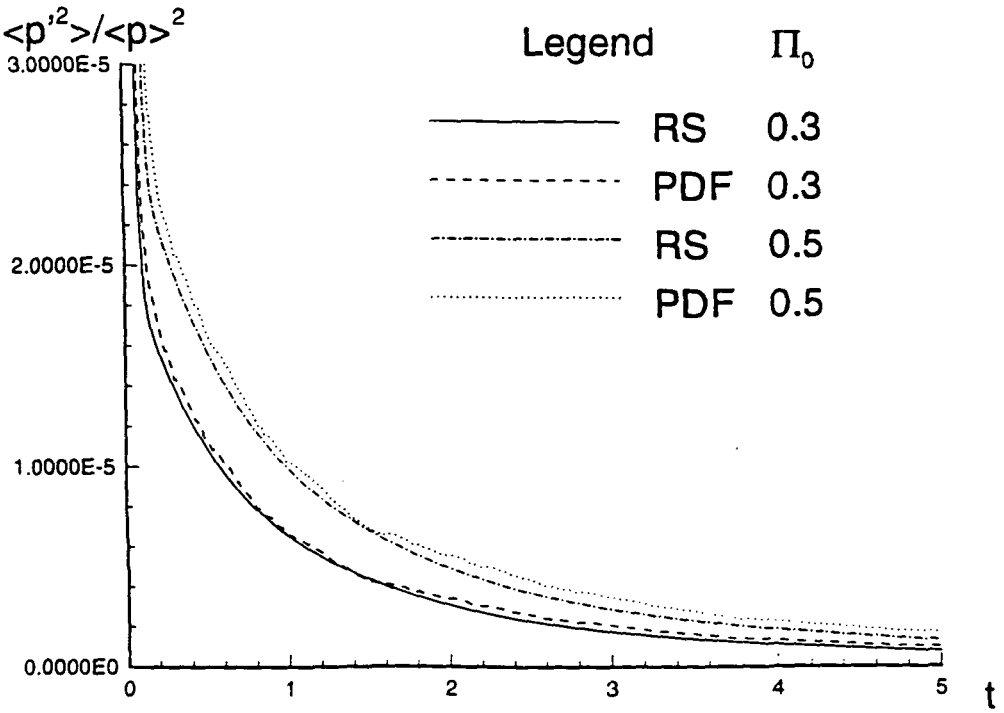

Fig. 2 (a). Comparison of normalized pressure variance values for the Reynolds stress closure (RS) and the PDF method (PDF). $M_{t0} = 0.05$, the values of Π_0 are given on the plot.

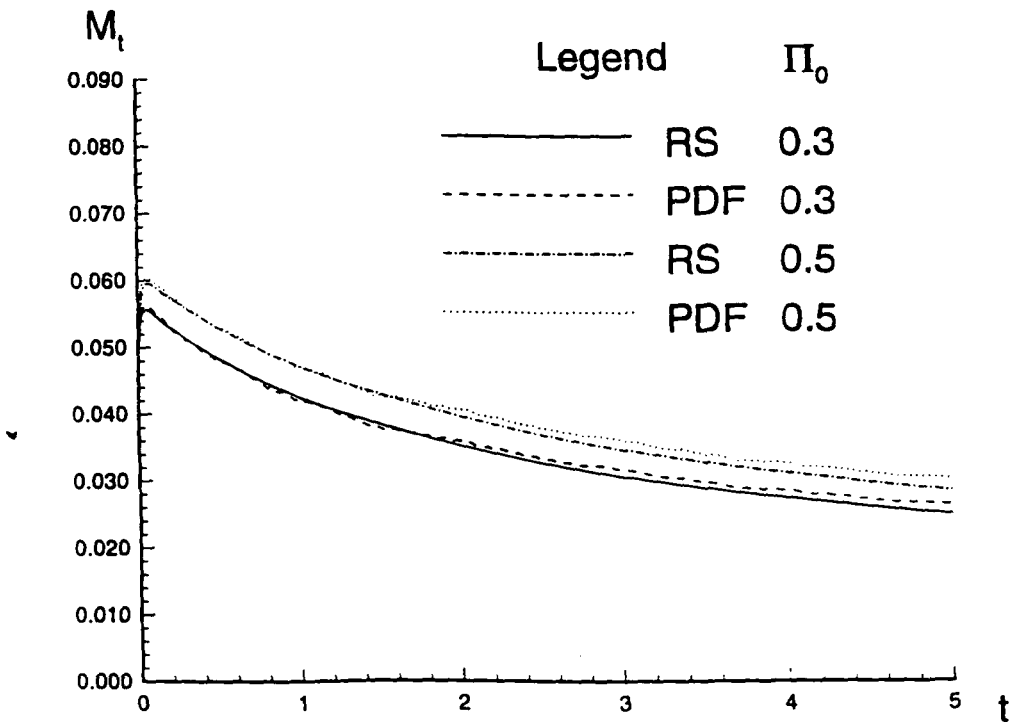

Fig. 2 (b). Comparison of turbulent Mach number values for the Reynolds stress closure (RS) and the PDF method (PDF). $M_{t0} = 0.05$, the values of Π_0 are given on the plot.

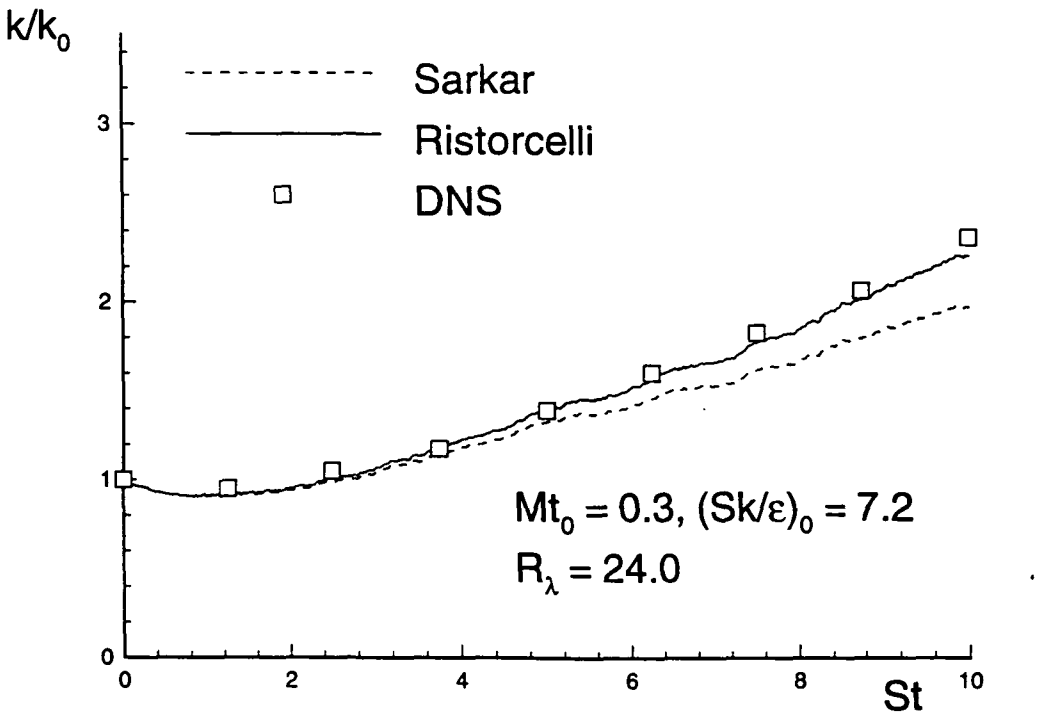

Fig. 3. Homogeneous shear flow: turbulence kinetic energy profiles using Zeman's model for the pressure-dilatation, and comparing Ristorcelli's model (Ristorcelli) and Sarkar's model (Sarkar) for the compressible dissipation.

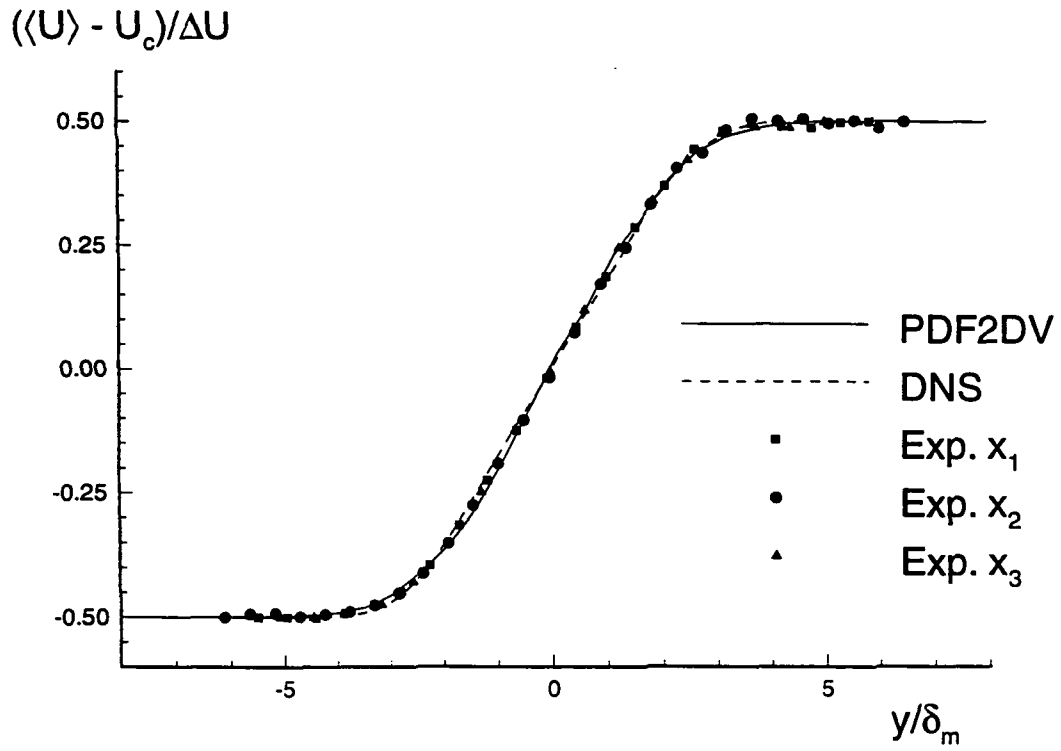

Fig. 4. Profiles of non-dimensional mean streamwise velocity vs. similarity coordinate. Solid line: PDF calculation; dashed line: DNS; symbols: experiments at 3 downstream locations.

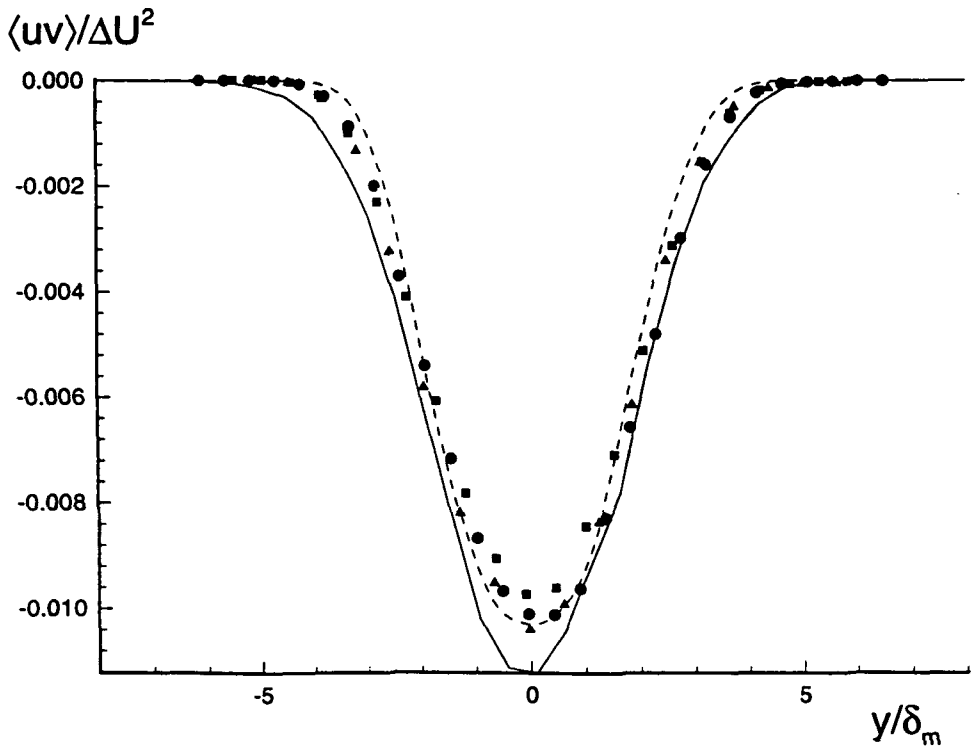

Fig. 5. Profiles of non-dimensional Reynolds shear stress vs. similarity coordinate. See fig. (4) for definitions.

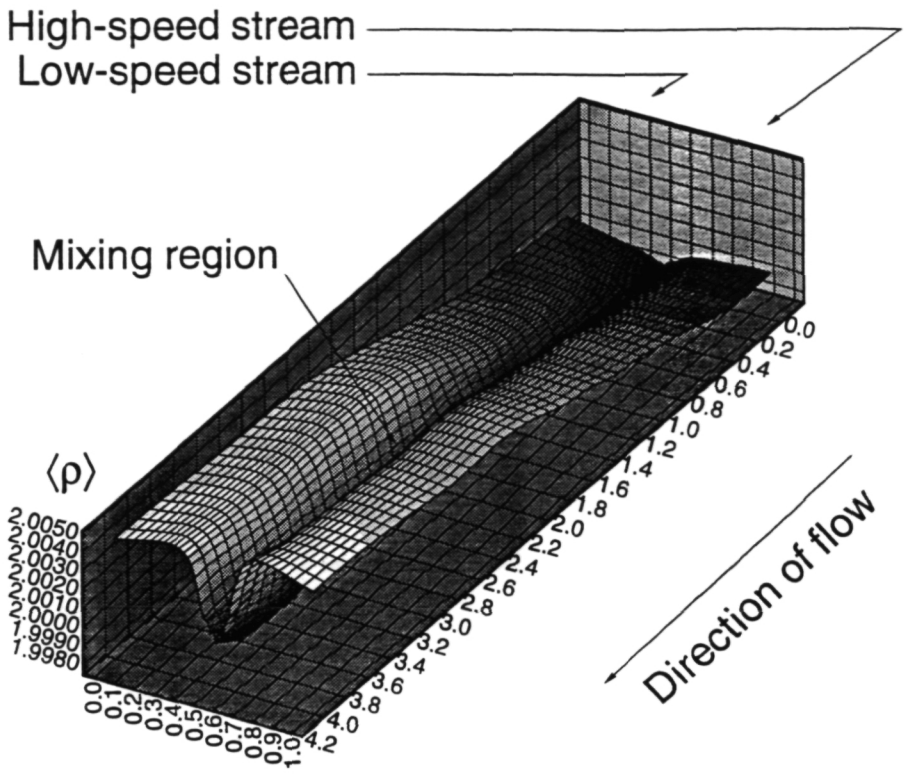

Fig. 6. Plane mixing layer: surface plot of mean density vs. streamwise and cross-stream coordinates.

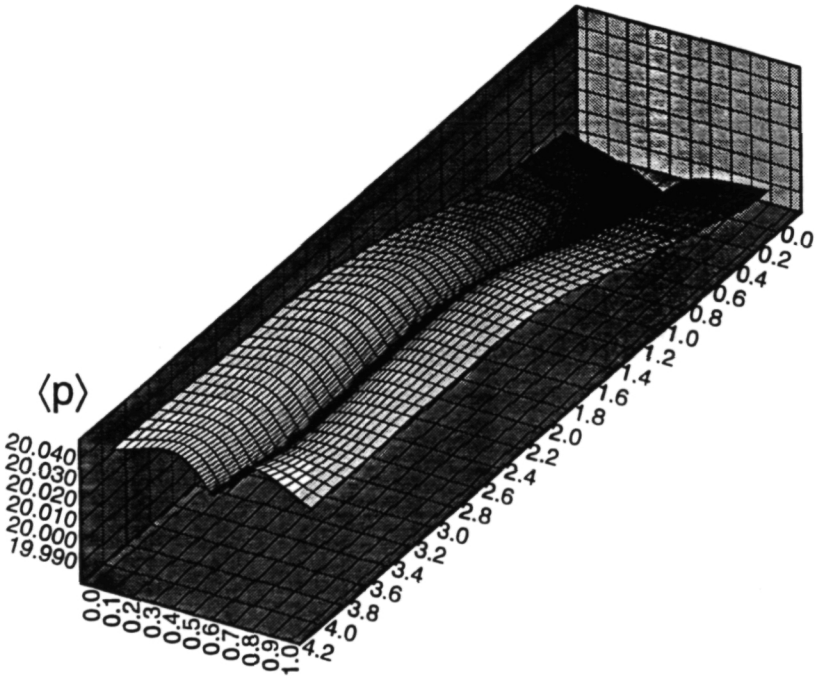

Fig. 7. Surface plot of mean pressure vs. streamwise and cross-stream coordinates.

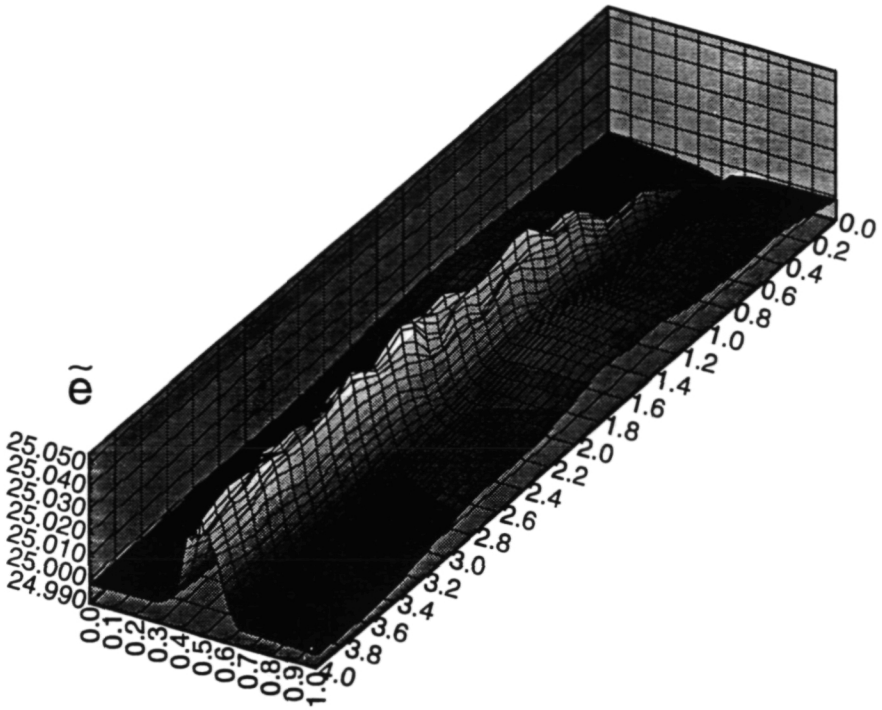

Fig. 6. Surface plot of mean internal energy vs. streamwise and cross-stream coordinates.

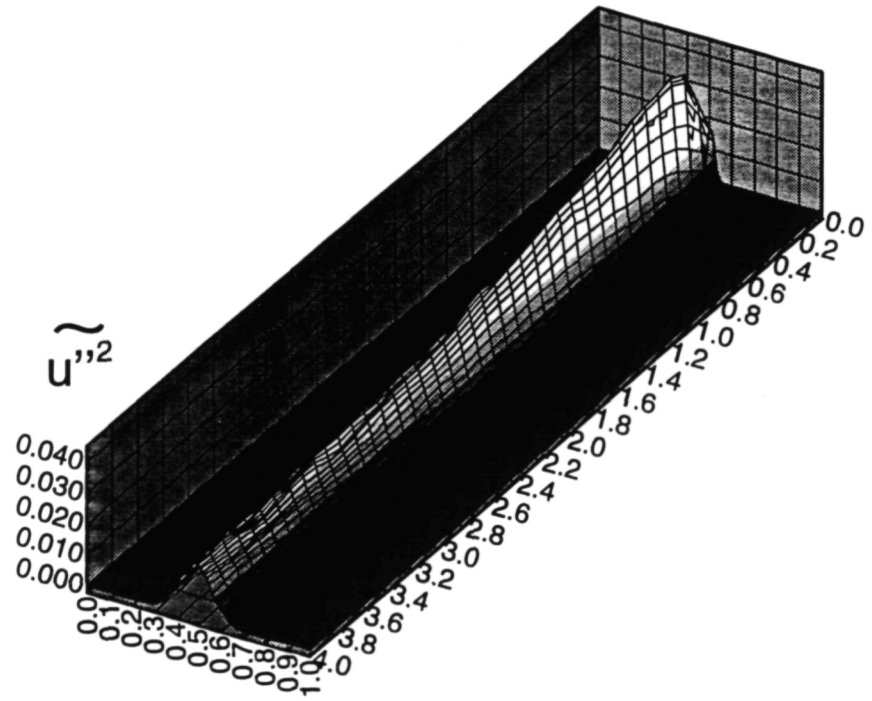

Fig. 7. Surface plot of streamwise turbulence intensity vs. streamwise and cross-stream coordinates. In our case the velocity difference across the layer is 1.